Crystal structure analysis of high temperature neutron diffraction data of novel oxide-ion conducting materials

Kotaro Fujii, Ayaka Fujimoto, Wataru Uno, Keigo Nakamura, Masatomo Yashima
Tokyo Institute of Technology

Oxide-ion conductors, which include pure ionic conductors and mixed oxide-ion and electronic conductors, attract significant interest because of their varied uses in oxygen separation membranes and cathodes for solid-oxide fuel cells (SOFCs). The oxide-ion conductivity is strongly dependent on the crystal structure. At present, several structures, such as fluorites, perovskites, K_2NiF_4, mellilites, and apatites, are known to show high oxide-ion conductivities. For further development of oxide-ion conductors is investigating materials with new types of structures. According to such background, we are exploring new structure family of oxide-ion conductors. For example, we have discovered a new structural family of oxide-ion conductor $NdBaInO_4$ which has a monoclinic $P2_1/c$ perovskite-related phase with a layered structure, in 2014. More recently, we found novel material, $SrRInO_4$ (R : rare earths) with $CaFe_2O_4$-type structure showed high oxide-ion conductivity compared to the other $CaFe_2O_4$-type materials. In order to understand the mechanism of oxide-ion conduction, it is necessary to precisely determine the crystal structure (particularly position, occupancy factor, and anisotropic displacement parameters of oxygens) at high-temperature because oxide-ion conductors are generally used at high-temperature. In the present study, we investigated the crystal structure of $SrRInO_4$ (R : rare earths) at high temperature using high resolution neutron powder diffractometer Echidna installed at the research reactor OPAL, ACNS, ANSTO. The materials were prepared by the solid-state reactions. The sintered pellets of the reaction products were introduced into a vanadium can and used for the neutron diffraction experiment. The measurements were carried out from room temperature to high temperature (1000 °C) at 200 °C intervals. Each measurement time was few hours. The structural analyses for these data are carried out by Rietveld method using the program RIETAN-FP. The result of the Rietveld refinement at the room temperature 23 °C is shown in Figure (R_{wp} =3.78 %, R_B = 3.82 %). For the diffraction data at 800 °C, the final Rietveld plot gave R_{wp} = 5.45 %, R_B = 6.35 % (see Figure for the fitting). Currently further structure analysis is ongoing.

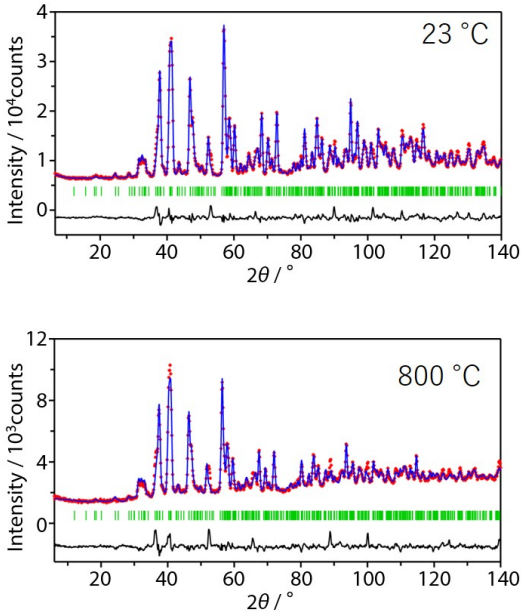

Fig. 1. Rietveld plots of SrRInO4 based material